Global chemistry-climate modelling with EMAC

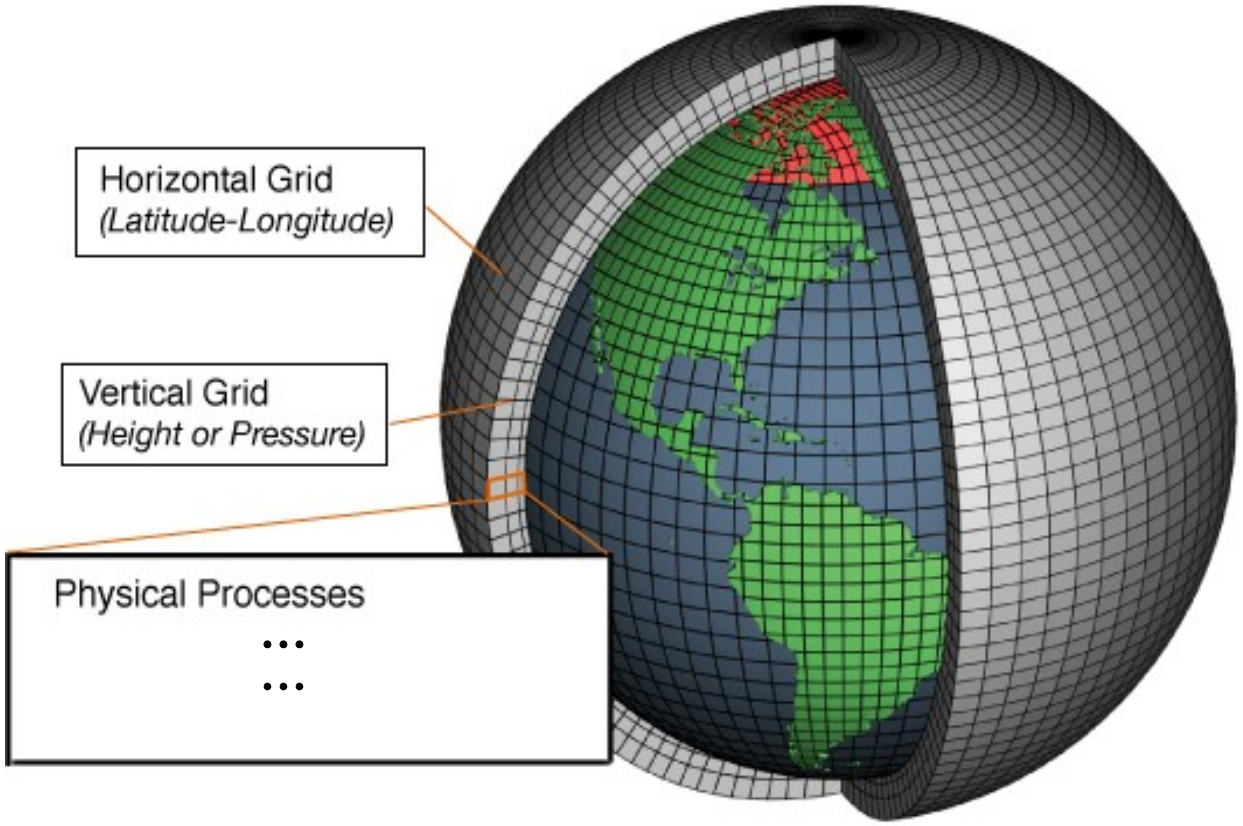
R. Deckert, R. Sausen, P. Jöckel, V. Aquila, S. Brinkop, U. Burkhardt,
I. Cionni, M. Dall'Amico, M. Dameris, S. Dietmüller, V. Eyring,
K. Gottschaldt, V. Grewe, J. Hendricks, M. Ponater, and M. Righi

Deutsches Zentrum für Luft- und Raumfahrt
Institut für Physik der Atmosphäre
Oberpfaffenhofen

High Performance Computing in Science and Engineering
Garching, 8 - 9 December 2009

Introduction

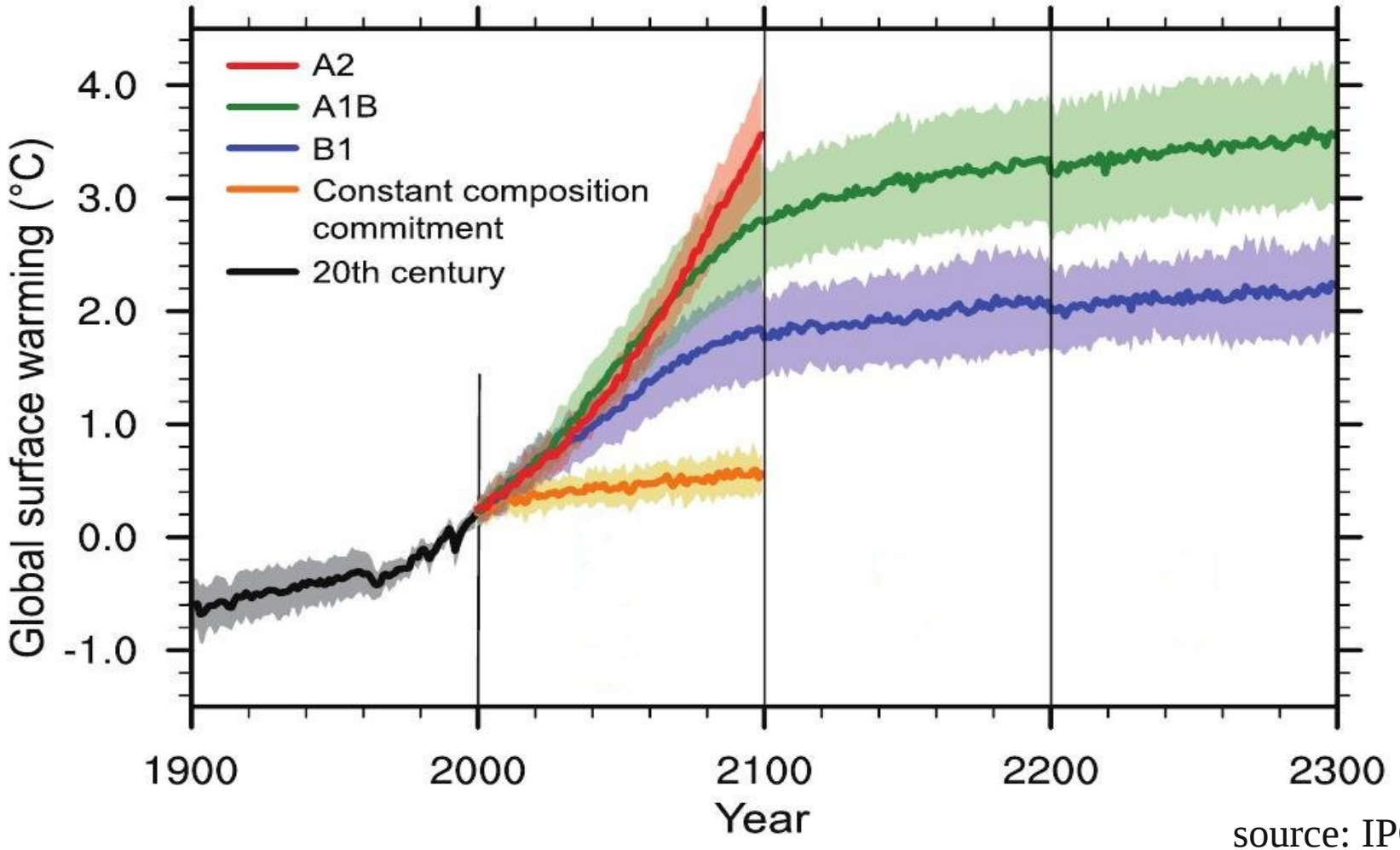
Global climate models



adapted from NOAA

Introduction

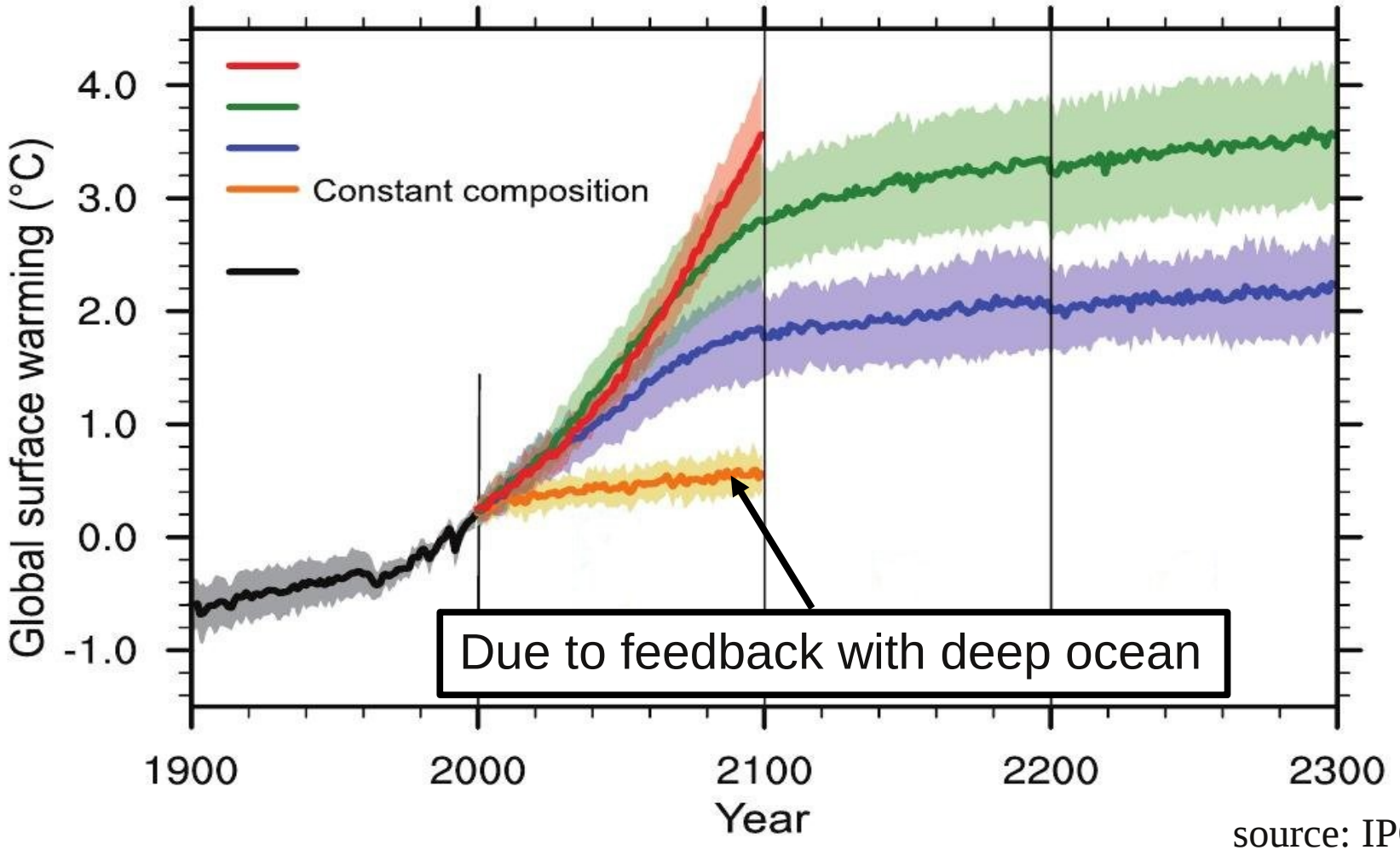
Global climate models: climate projections



source: IPCC

Introduction

Global climate models: climate projections



source: IPCC

Introduction

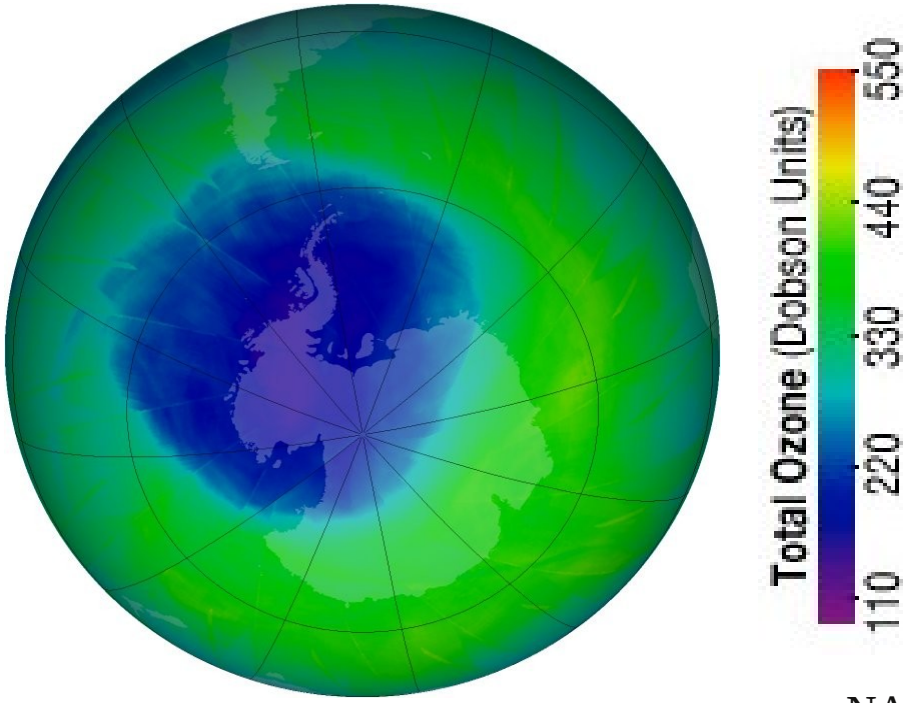
Global climate models: no atmospheric chemistry

Introduction

Global climate models: no atmospheric chemistry

- Future ozone layer?

21st November 2009



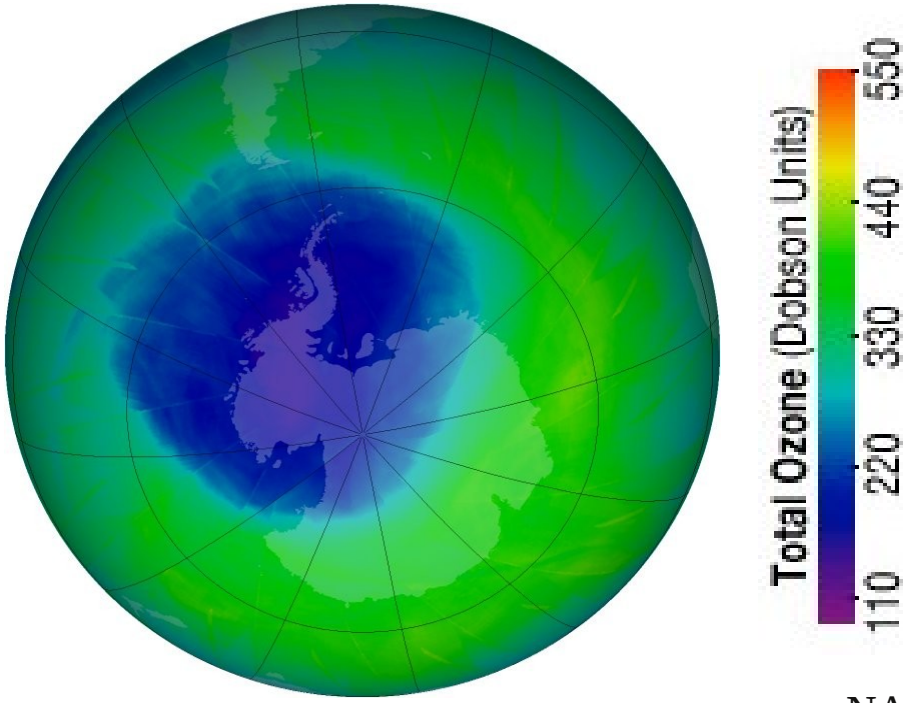
source: NASA

Introduction

Global climate models: no atmospheric chemistry

- Future ozone layer?
- Chemically triggered climate modifications?

21st November 2009



source: NASA

Introduction

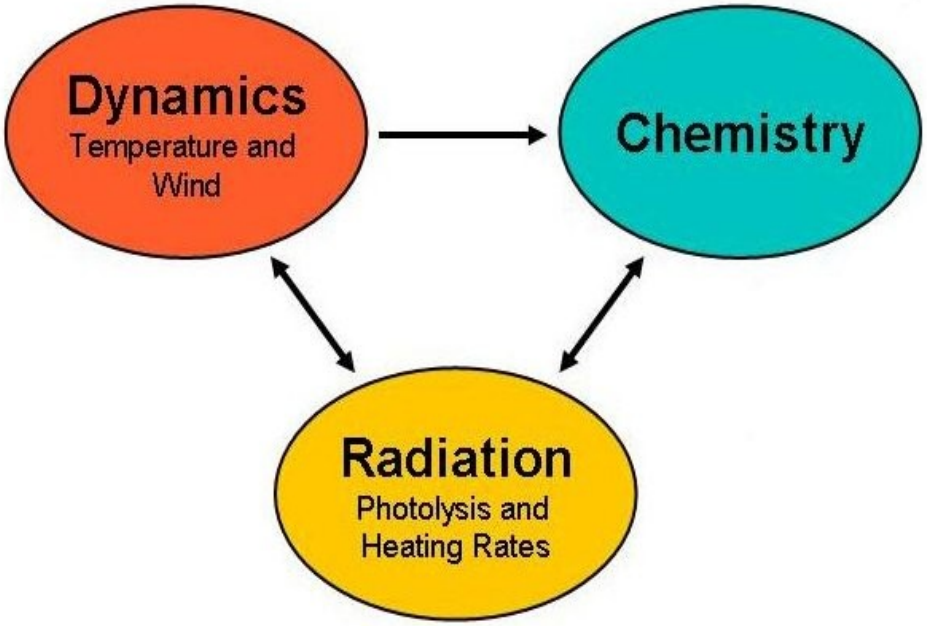
Global chemistry-climate models (CCMs)

- Atmosphere ~~<~~ deep ocean

Introduction

Global chemistry-climate models (CCMs)

- Atmosphere ~~↔~~ deep ocean
- Atmospheric physics ↔ atmospheric chemistry

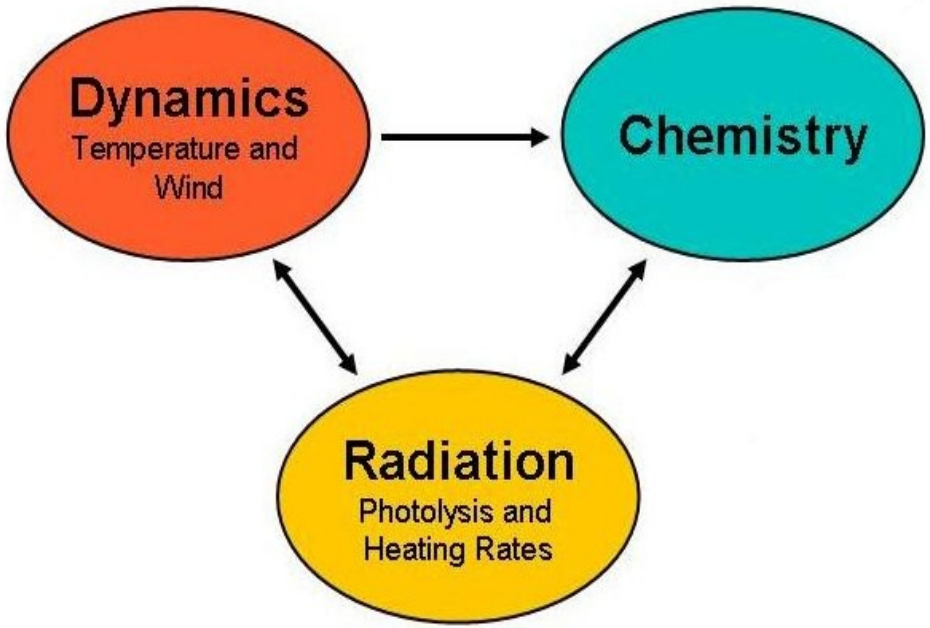


Introduction

Global chemistry-climate models (CCMs)

- Atmosphere ~~⇎~~ deep ocean
- Atmospheric physics ↔ atmospheric chemistry

We use and refine a CCM



Outline

- Model description
- Performance on LRZ/ALTIX
- Modelling activities on LRZ/ALTIX

Description

CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg

Description

CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg

EMAC follows standards → easily portable

- Fortran95 (ISO/IEC-1539-1)
- Message Passing Interface (MPI-2)
- NetCDF data format

Description

CCM system EMAC (ECHAM/MESSy Atmospheric Chemistry)

- Overall system by MPI for Chemistry, Mainz
- Fluid dynamics by MPI for Meteorology, Hamburg

EMAC follows standards → easily portable

- Fortran95 (ISO/IEC-1539-1)
- Message Passing Interface (MPI-2)
- NetCDF data format

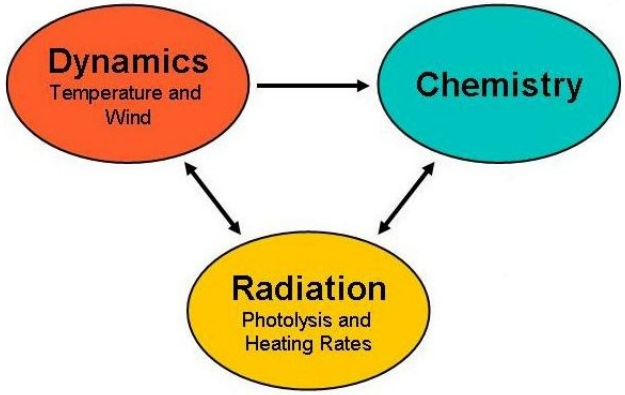
EMAC is flexible

- Selectable spatial resolution
- Configurable chemistry scheme
- Modular structure (see *http://www.messy-interface.org*)

Description

Atmospheric primitive equations − spectral representation

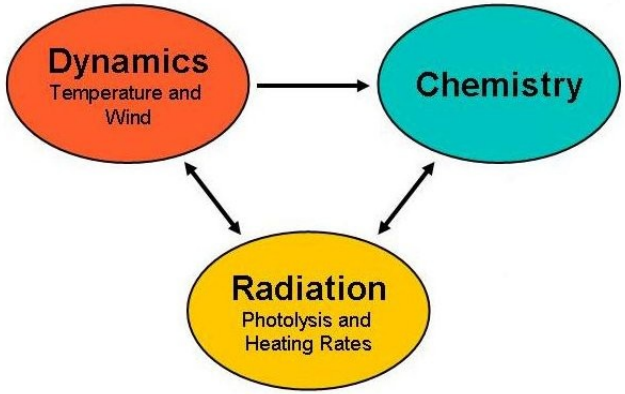
- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)



Description

Atmospheric primitive equations − spectral representation
- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)

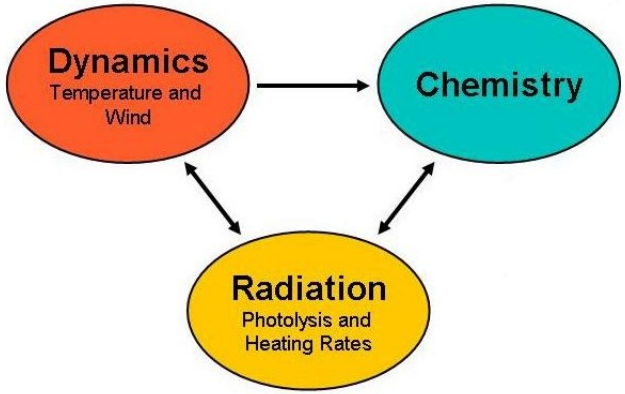
Stiff system of ordinary differential equations − gaussian grid
Rosenbrock sparse-matrix technique with adaptive time step



Description

Atmospheric primitive equations − spectral representation
- Spectral transformation (horizontal)
- Finite differences (vertical)
- Semi-implicit leap frog (time)

Stiff system of ordinary differential equations − gaussian grid
Rosenbrock sparse-matrix technique with adaptive time step



Radiative transfer, tracer transport, other sub-models – gaussian grid
Miscellaneous techniques

Description

Diverse demands on hardware architecture ...

- Various numerical techniques

Description

Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
  - Spectral representation: spherical
  - Gaussian grid: latitude-longitude, ping-pong blocks
  - Tracer advection: vertical and latitude-longitude

Description

Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
  - Spectral representation: spherical
  - Gaussian grid: latitude-longitude, ping-pong blocks
  - Tracer advection: vertical and latitude-longitude
- Vectorisation of latitude-longitude blocks
  - To exploit cache sizes

Description

Diverse demands on hardware architecture ...

- Various numerical techniques
- Distributed-memory domain decomposition
  - Spectral representation: spherical
  - Gaussian grid: latitude-longitude, ping-pong blocks
  - Tracer advection: vertical and latitude-longitude
- Vectorisation of latitude-longitude blocks
  - To exploit cache sizes

→ EMAC valuable for benchmarking

Performance on LRZ/ALTIX

Good performance, but gain limited

EMAC with detailed physics/chemistry

vertical layers	*CPUs*	*CPU time [kh/model year]*	*wall time [days/model year]*
L41	***64***	**5.4**	**3.5**
L41	***128***	**7.9**	**2.6**
L90	***64***	**12.0**	**7.9**
L90	***128***	**12.1**	**4.0**
L90	***256***	**poor**	**poor**

Performance on LRZ/ALTIX

Good performance, but gain limited

- Communication between nodes (hardware specific)

EMAC with detailed physics/chemistry

vertical layers	*CPUs*	*CPU time [kh/model year]*	*wall time [days/model year]*
L41	***64***	**5.4**	**3.5**
L41	***128***	**7.9**	**2.6**
L90	***64***	**12.0**	**7.9**
L90	***128***	**12.1**	**4.0**
L90	***256***	**poor**	**poor**

Performance on LRZ/ALTIX

Good performance, but gain limited

- Communication between nodes (hardware specific)
- Load imbalance from photo-chemistry (being tackled)

EMAC with detailed physics/chemistry

vertical layers	*CPUs*	*CPU time [kh/model year]*	*wall time [days/model year]*
L41	***64***	**5.4**	**3.5**
L41	***128***	**7.9**	**2.6**
L90	***64***	**12.0**	**7.9**
L90	***128***	**12.1**	**4.0**
L90	***256***	**poor**	**poor**

Performance on LRZ/ALTIX

Good performance, but gain limited

- Communication between nodes (hardware specific)
- Load imbalance from photo-chemistry (being tackled)

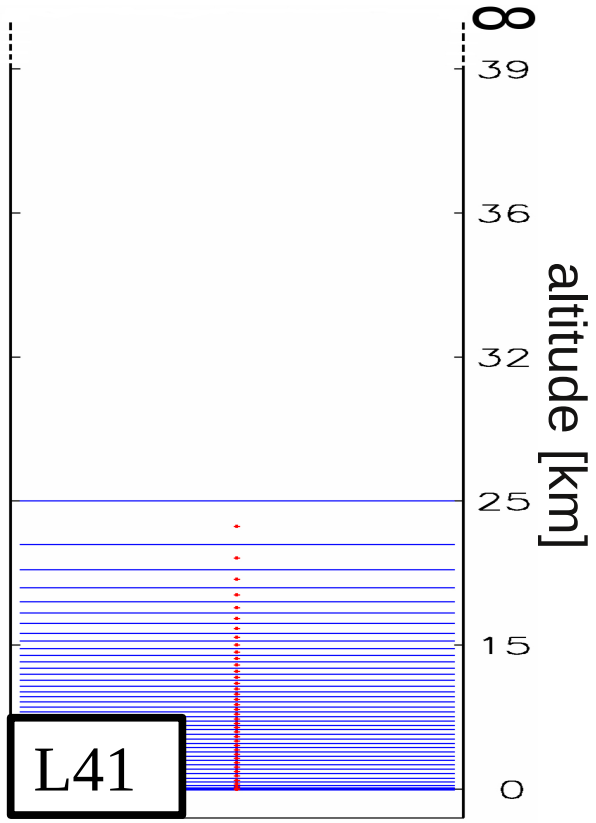
L41 version: multi-decadal simulations sensible

EMAC with detailed physics/chemistry

vertical layers	*CPUs*	*CPU time [kh/model year]*	*wall time [days/model year]*
L41	***64***	**5.4**	**3.5**
L41	***128***	**7.9**	**2.6**
L90	***64***	**12.0**	**7.9**
L90	***128***	**12.1**	**4.0**
L90	***256***	**poor**	**poor**

Development: new upper boundary

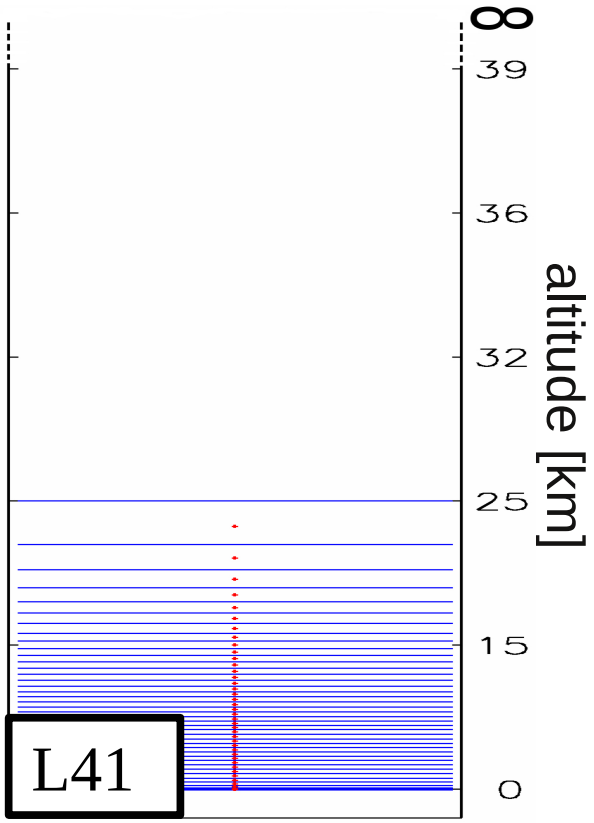
L90 expensive → our L41 version



Development: new upper boundary

L90 expensive → our L41 version

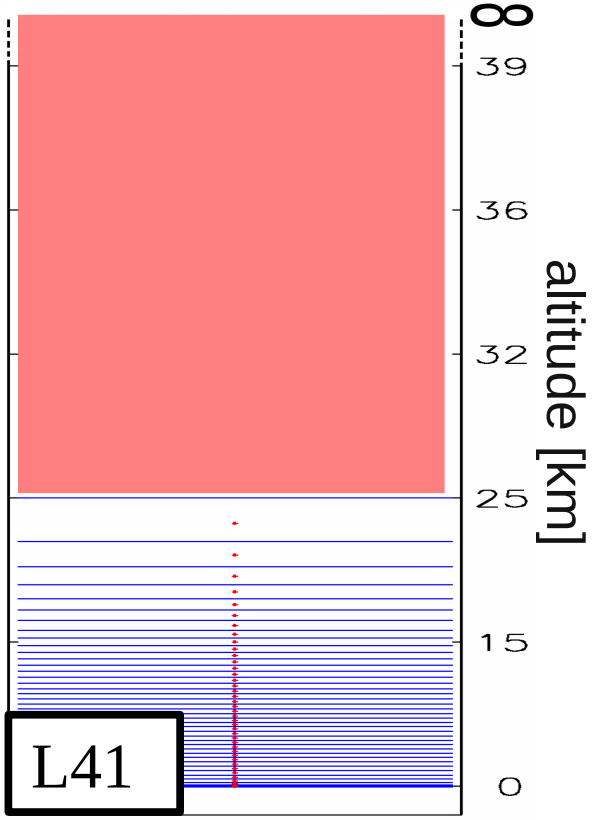
- Appropriate for our purposes



Development: new upper boundary

L90 expensive → our L41 version

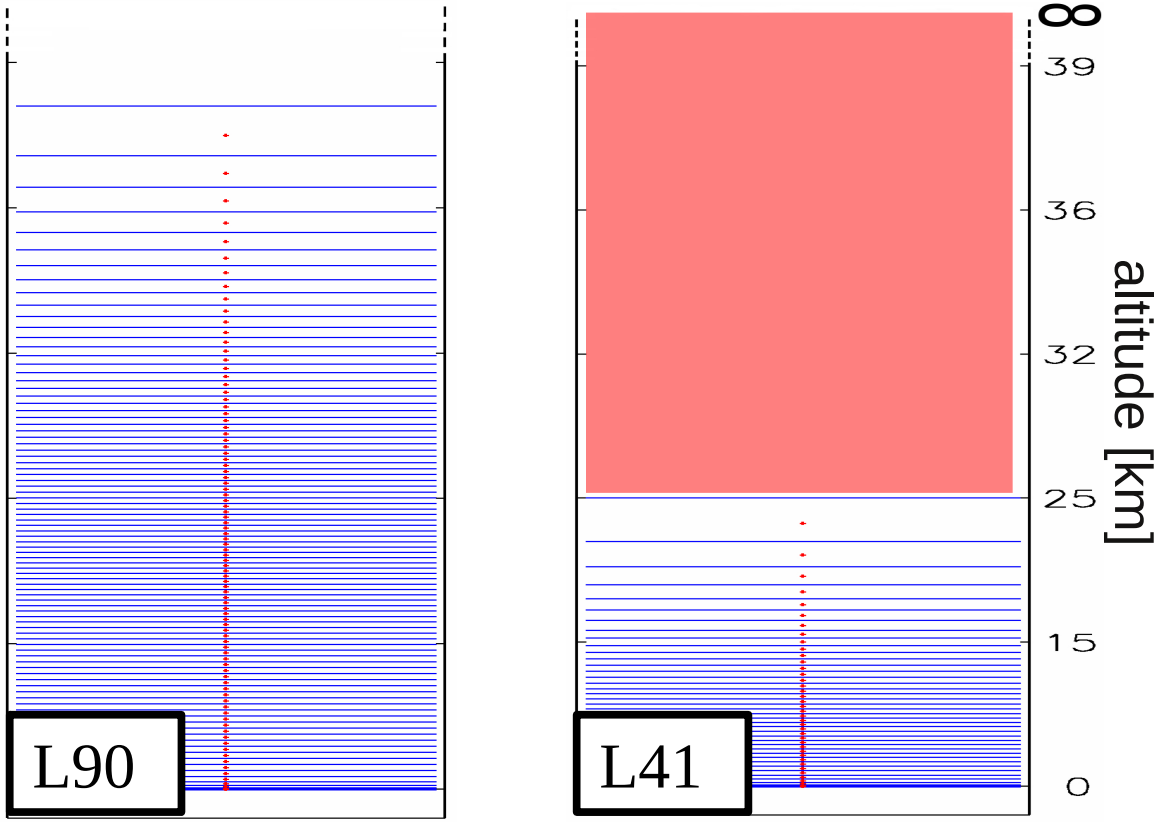
- ➢ Appropriate for our purposes
- ➢ But: single layer for whole atmosphere above 25 km
- → Impact on chemistry below



Development: new upper boundary

Solution: highest layer with chemical parameterisation

- Calibration via L90 version



Development: new upper boundary

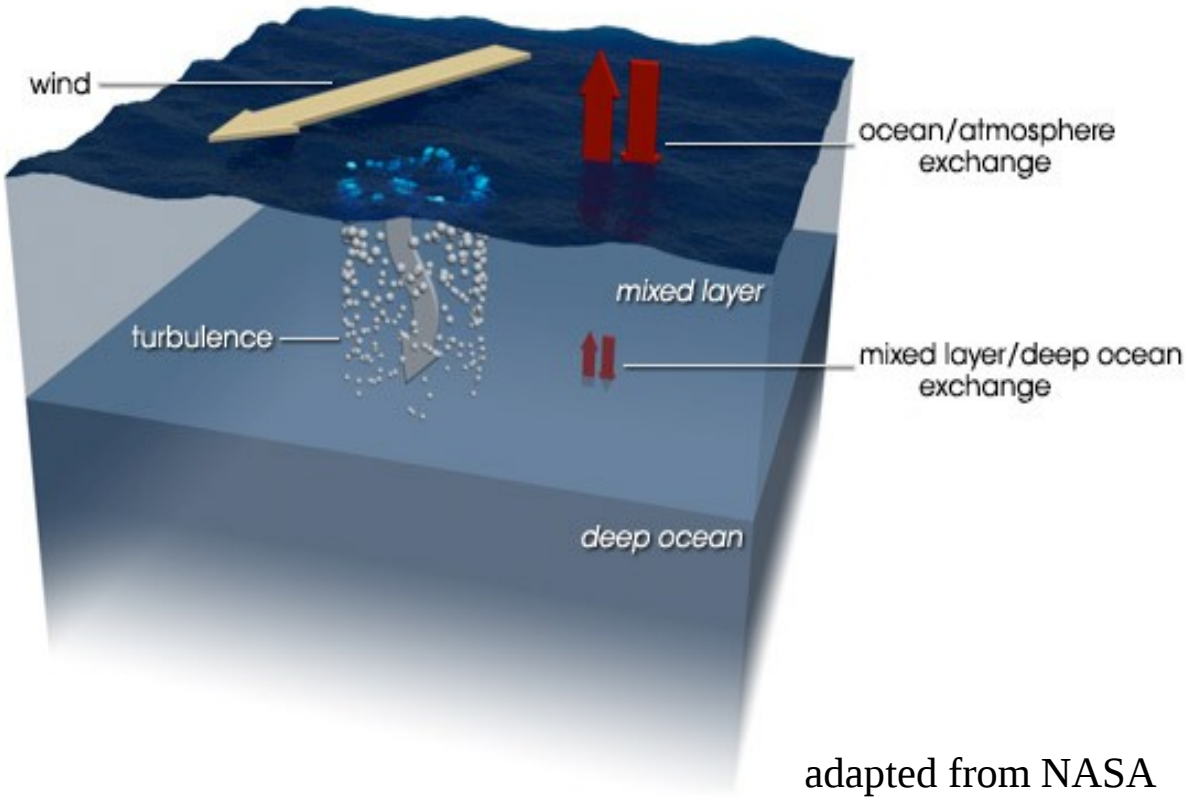
Solution: highest layer with chemical parameterisation

- Calibration via L90 version

Development: mixed-layer ocean

Implementation of mixed-layer ocean

- Feedback: atmosphere ↔ mixed-layer ocean
- No feedback: mixed-layer ocean ↔ deep ocean



adapted from NASA

Development: mixed-layer ocean

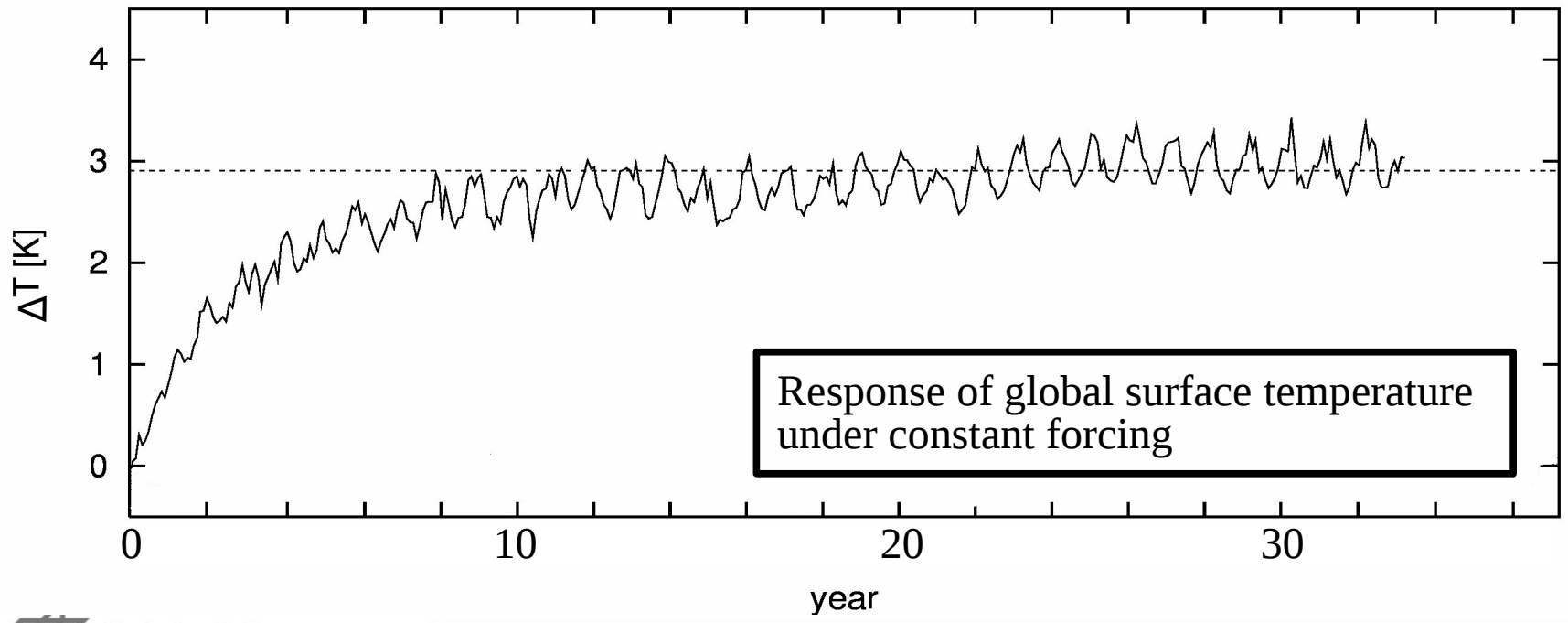
Mixed-layer ocean – additional computational demands

- Negligible for fix simulation length

Development: mixed-layer ocean

Mixed-layer ocean – additional computational demands

- Negligible for fix simulation length
- However: spin-up about twenty years
- Much longer for deep ocean

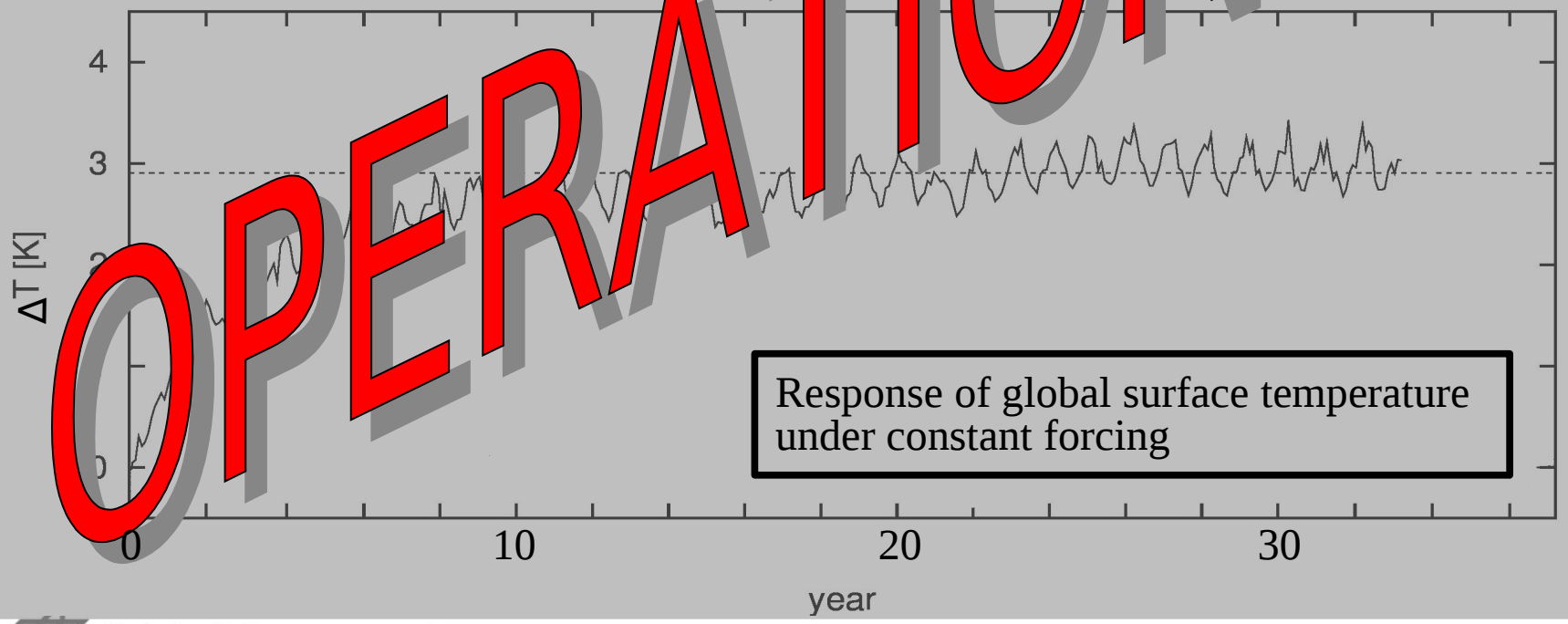


Development: mixed-layer ocean

Mixed-layer ocean – additional computational demands

- Negligible for fix simulation length
- However: spin-up about twenty years
- Much longer for deep ocean

OPERATIONAL



Development: Lagrangian formulation

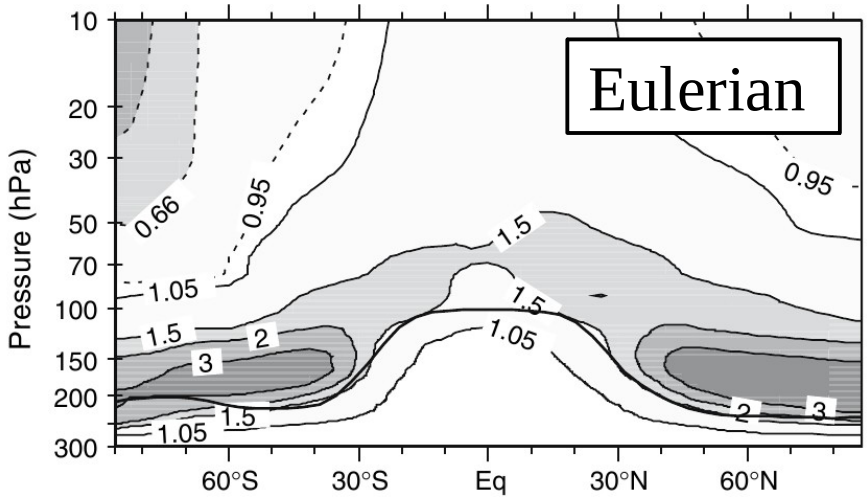
Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive



Water vapour: ratio EMAC/satellite

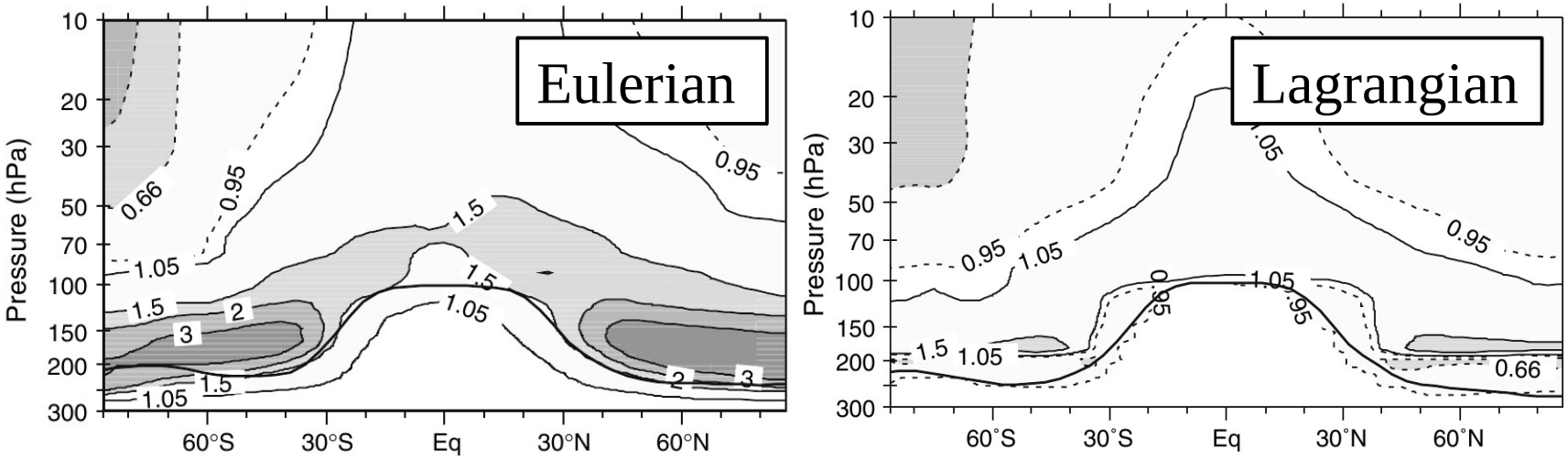
Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangian tracer transport

- No numerical diffusion



Water vapour: ratio EMAC/satellite

Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangian tracer transport

- No numerical diffusion

OPERATIONAL

Development: Lagrangian formulation

Standard formulation of fluid dynamics: Eulerian

- Separate schemes for dynamics and tracer transport
- Tracer transport numerically diffusive

Implementation of full-Lagrangian tracer transport

- No numerical diffusion

In development: full-Lagrangian dynamical core

- Finite-mass method (Gauger et al., 2000)
- Lagrangain air parcels with variable spatial extent
- Completely new approach in climate modelling

Development: chemistry-transport mode

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- E.g. human-made nitrogen oxide → near-surface ozone

Development: chemistry-transport mode

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- E.g. human-made nitrogen oxide → near-surface ozone

Usually: difference of CCM simulations with un-/disturbed emission rates

- Noise from dynamical-chemical feedback
- Poor signal/noise ratio

Development: chemistry-transport mode

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- E.g. human-made nitrogen oxide → near-surface ozone

Usually: difference of CCM simulations with un-/disturbed emission rates

- Noise from dynamical-chemical feedback
- Poor signal/noise ratio

Our solution: switch off feedback

- Dynamics binary identical despite chemistry unequal
- Main challenge: polar stratospheric clouds

Development: chemistry-transport mode

Important question

- Impact of disturbed emission rates on atmospheric composition and climate
- E.g. human-made nitrogen oxide → near-surface ozone

Usually: difference of CCM simulation with an-/disturbed emission rates

- Noise from dynamical-chemical feedback
- Poor signal/noise ratio

Our solution: switch off feedback

- Dynamics combination identical despite chemistry unequal
- Main challenge: polar stratospheric clouds

OPERATIONAL

Production simulations

Focus on model development:
prerequisite for production simulations

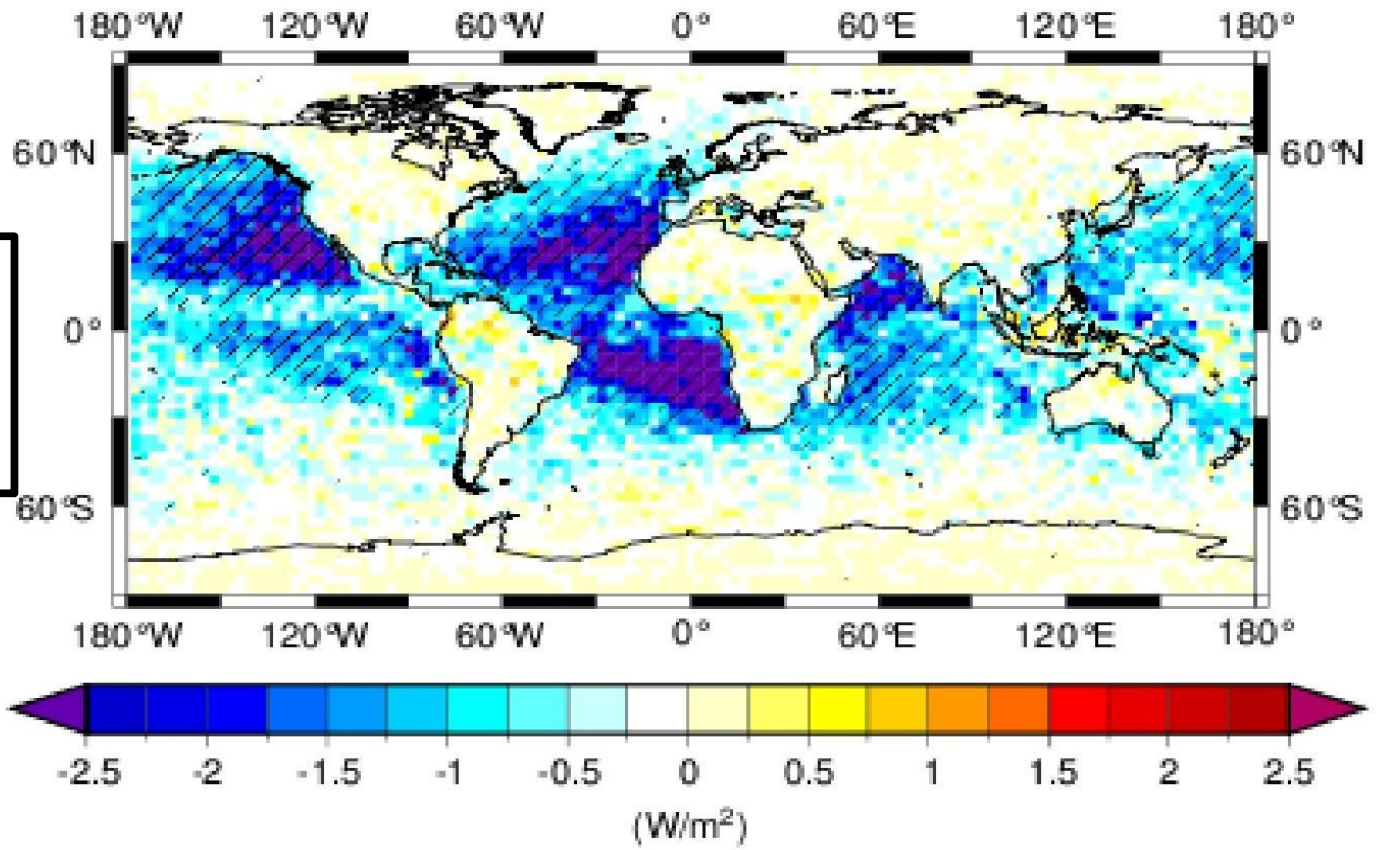
→ Now feasible and going to start

Production simulations

Climate impact of nitrogen oxide and sulfur dioxide from shipping

- Affects optical and microphysical cloud properties
- Mostly cooling

Short-wave forcing du to ship emissions

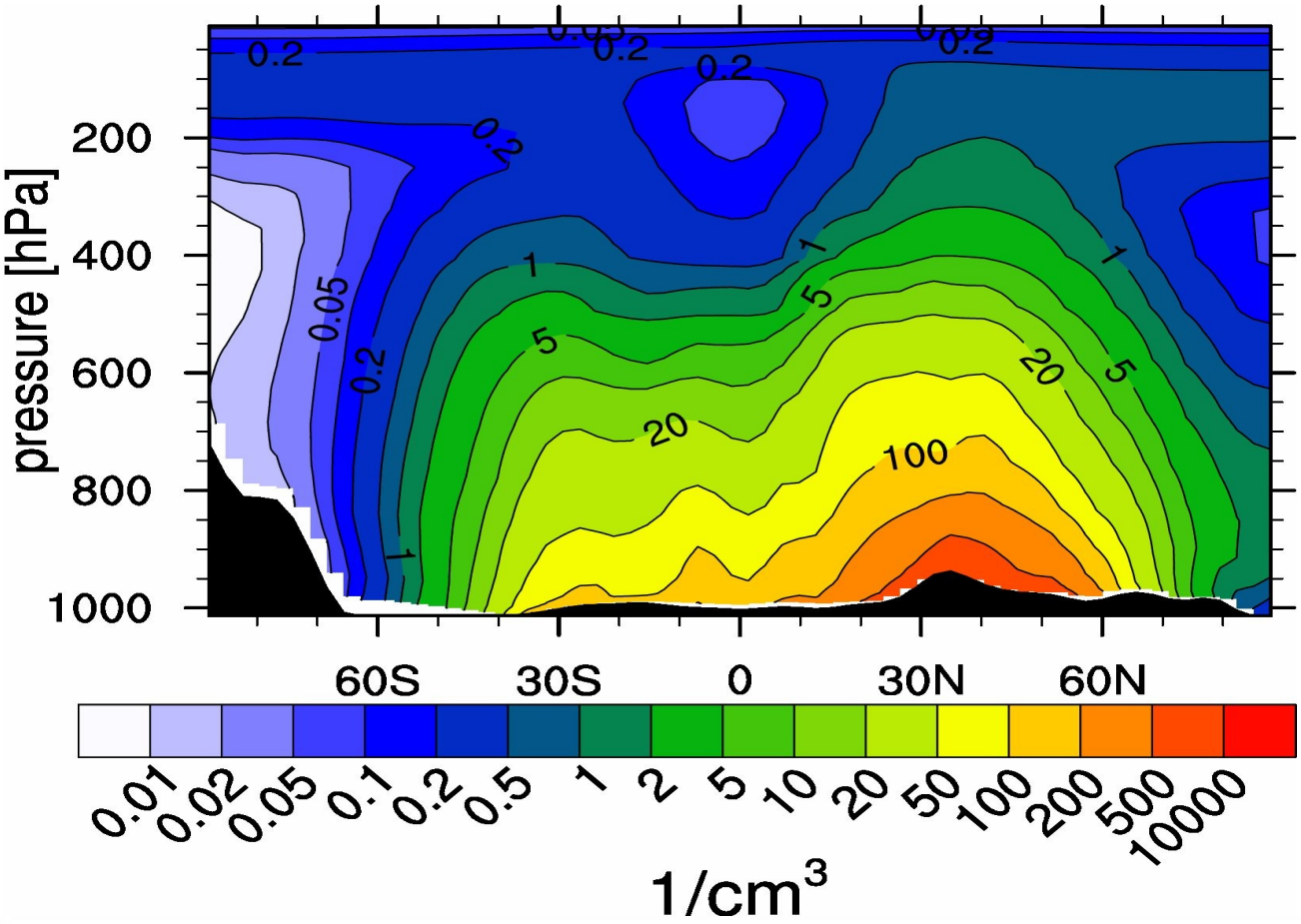


Production simulations

Aerosol aging

- ➢ Can result in ice nuclei

→ Affects cirrus clouds



Number concentration of potential ice nuclei

Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes

Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes

Model development ...

- New upper boundary
- Mixed-layer ocean
- Lagrangian transport
- Chemistry-transport mode

Summary

We use a chemistry-climate model (CCM)

- Diverse numerics / types of domain decomposition
- Good performance on LRZ/ALTIX
- But: gain limited due to communication between nodes

Model development ...

- New upper boundary
- Mixed-layer ocean
- Lagrangian transport
- Chemistry-transport mode

→ **Production going to start**